Aalto-yliopisto
Perustieteiden korkeakoulu

Machine learning for unconventional superconductivity (finished)

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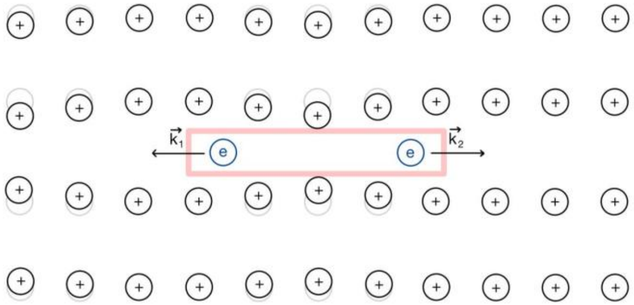
Goals & scope

- Superconductivity = total loss of electrical resistance in a material
- Goal: building a neural network model able to recognise unconventional (topological) superconductivity from real space conductance measurements
- Requires a significant amount of features (inputs) and data points

Recap: Superconductivity

- Superconducting can happen when electrons pass through the lattice of a metal
  - The vibrations of ions in a lattice cause an **attractive interaction** between electrons
  - Vibrations are waves, and quanta of these vibrations are quasi-particles
    - Conventional superconductivity: phonons
    - **Unconventional superconductivity**: phonons or other quasi-particles

- A superconducting state is described through **Cooper pairs**
  - The attractive **interaction** between electrons causes a paired state of electrons to have energy lower than the Fermi energy
    → bound state of a pair of electrons



Recap: Mathematical representation of superconductivity

- Superconducting states represented with Hamiltonians (total energy operators):

$$H = \sum_{ij} t_{ij}(c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}) + \sum_{i} U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}$$

- $c_{ns}^{\dagger}$ and c_{ns} are the creation and annihilation operators, respectively
- t_{ij} represents hopping between sites i and j (kinetic energy gained or lost)
- U is the interaction term, with U<0 for superconductivity

- Four fermion model is not solvable
  – approximated using two fermions:

$$H \approx \sum_{ij} t_{ij}(c_{i\uparrow}^{\dagger} c_{j\uparrow} + c_{i\downarrow}^{\dagger} c_{j\downarrow}) + \sum_{i} \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle c_{i\uparrow} c_{i\downarrow} + h.c.$$

Where $\Delta = \langle c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} \rangle$ is the superconducting order

Background: topological superconductivity

- Unconventional superconductors with unique and stable quantum properties
- Protected by the material's shape and structure (topology) at a microscopic level
  - able to carry information without losing it due to noise
  - potential candidates for robust quantum computing applications
- A conventional s-wave superconductor can be turned into a topological superconductor by introducing an exchange field and Rashba spin-orbit coupling (SOC)

$$H_J = J_z \sum_{i,s,s'} \sigma_z^{s,s'} c_{i,s}^\dagger c_{i,s'} \qquad H_R = i\lambda_R \sum_{\langle ij \rangle, ss'} d_{ij} \cdot \sigma^{s,s'} c_{i,s}^\dagger c_{j,s'}$$

- J_z is the exchange coupling
- σ are spin Pauli matrices
- λ_R is Rashba spin-orbit coupling (SOC)

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Recap: Measuring Superconductivity

- Superconducting states are of the form $\langle c^\dagger_{\uparrow i} c^\dagger_{\downarrow i} \rangle = f(k)$ where $f(k)$ is a pairing between particles and $c^\dagger_{\uparrow i}$
- This cannot be directly measured
- Materials can be imaged at the atomic level using scanning tunnelling microscopy (STM)
  - Differential conductance dI/dV can be obtained
  - This reveals the electronic structure and the pairing mechanism
  - Called the density of states (DOS) of the system

Simulating a topological superconductor

- The Hamiltonian is defined as

$$H = H_{kin} + H_R + H_J + H_{SC}$$

- μ is the chemical potential energy

where

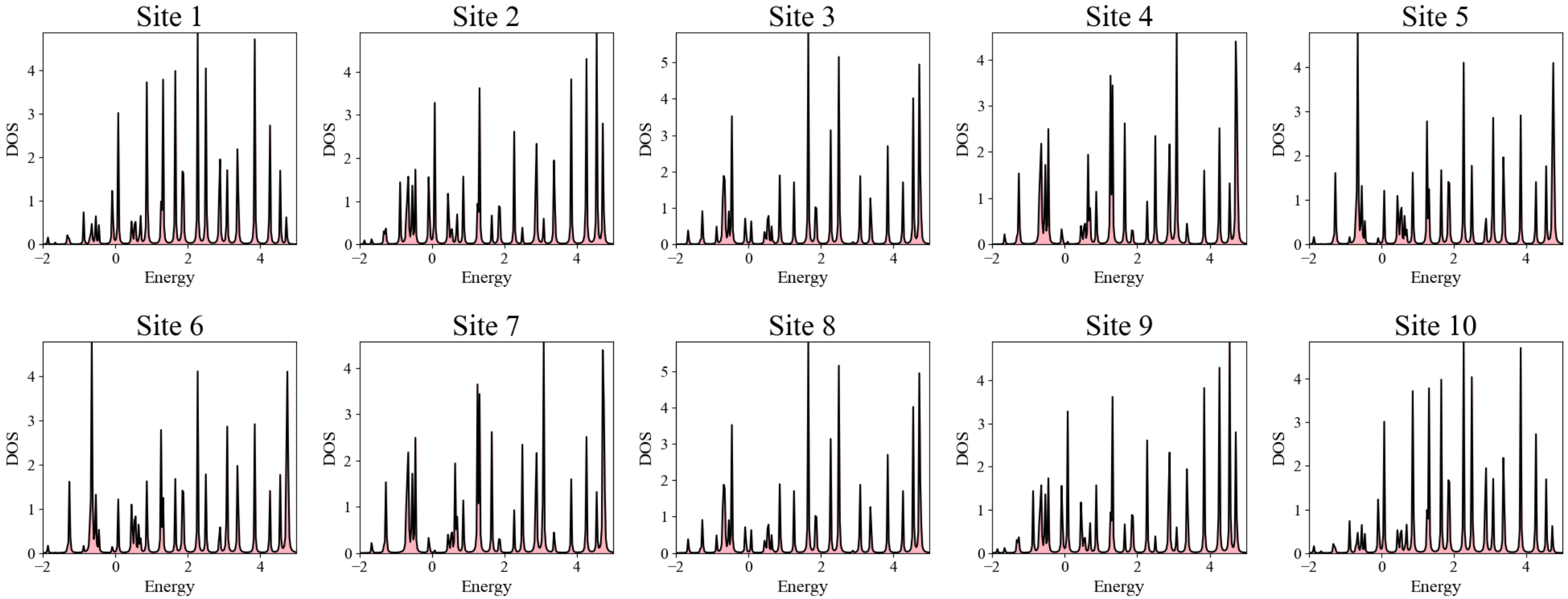
$$H_{kin} = \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} \qquad H_J = J_z \sum_{i,s,s'} \sigma_z^{s,s'} c_{i,s}^\dagger c_{i,s'}$$

$$H_R = i\lambda_R \sum_{\langle ij \rangle, ss'} d_{ij} \cdot \sigma^{s,s'} c_{i,s}^\dagger c_{j,s'} \qquad H_{SC} = \sum_i \Delta c_{i\uparrow} c_{i\downarrow} + h.c.$$

- A set of Hamiltonians is created with different Δ, J_z, λ_R values using Python-library pyqula
  - **Δ, J_z, λ_R are the outputs** of the model

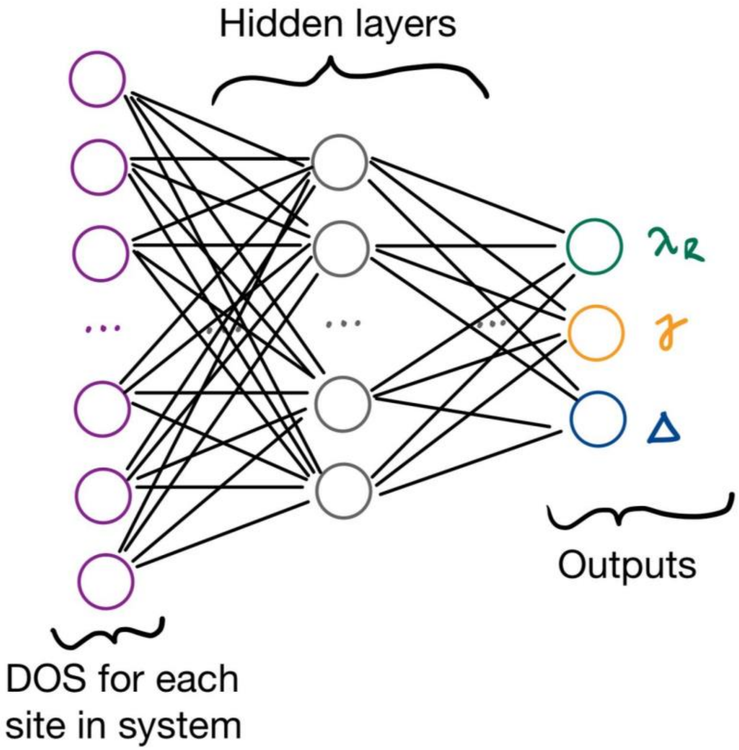
Simulating a topological superconductor

- DOS is computed for each site of each Hamiltonian
  - Results in DOS values in the amount of n.o. sites in system multiplied by the n.o. energies the DOS is measured for
  - **DOS values are the inputs** of the model

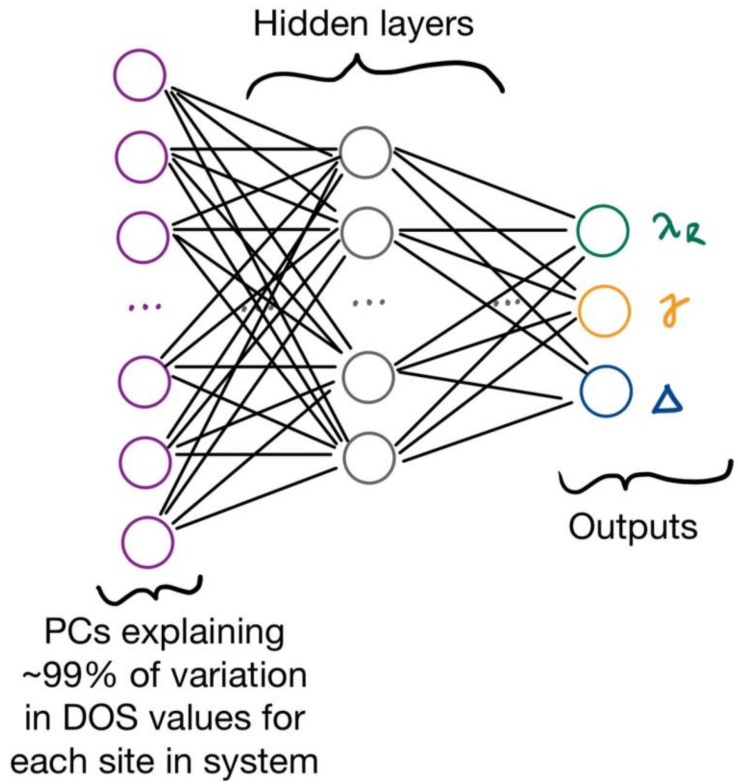


Neural network models

- DOS values as input



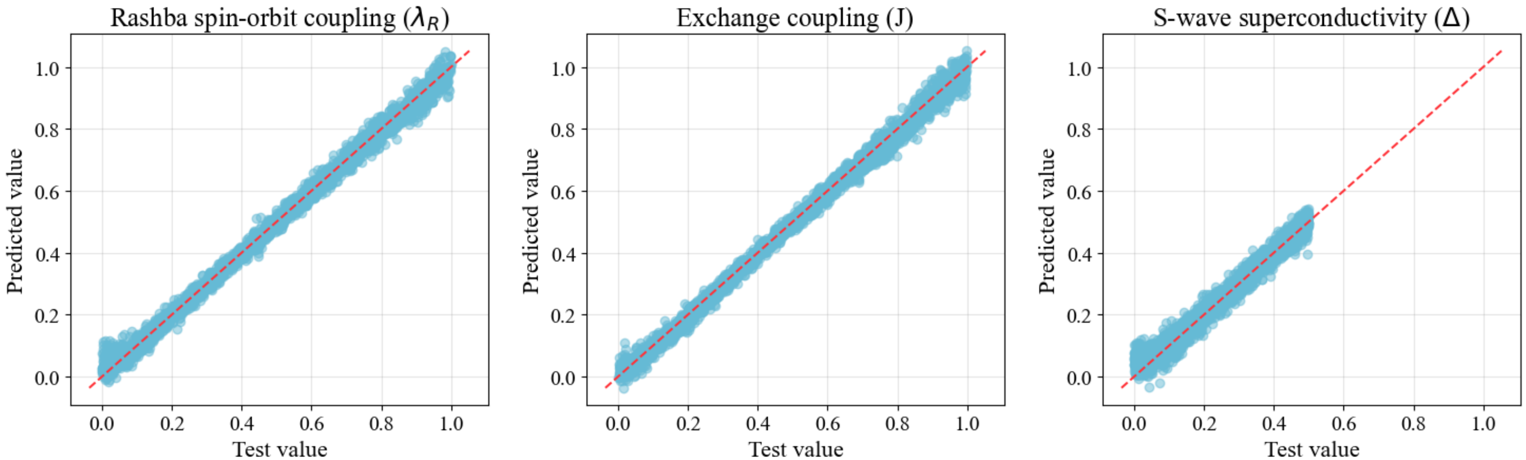
- PCs as input

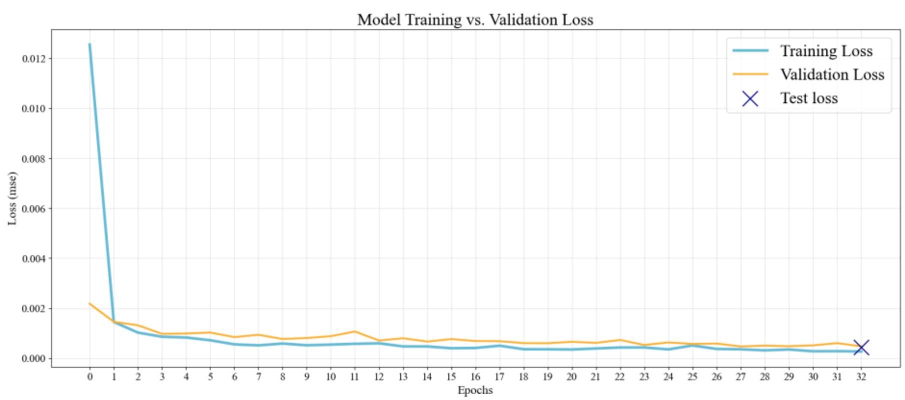


RESULTS

10 site system

No data compression: input space of size 2500,
10 000 Hamiltonians, 20/80 split





10 site system

No data compression: input space of size 2500,
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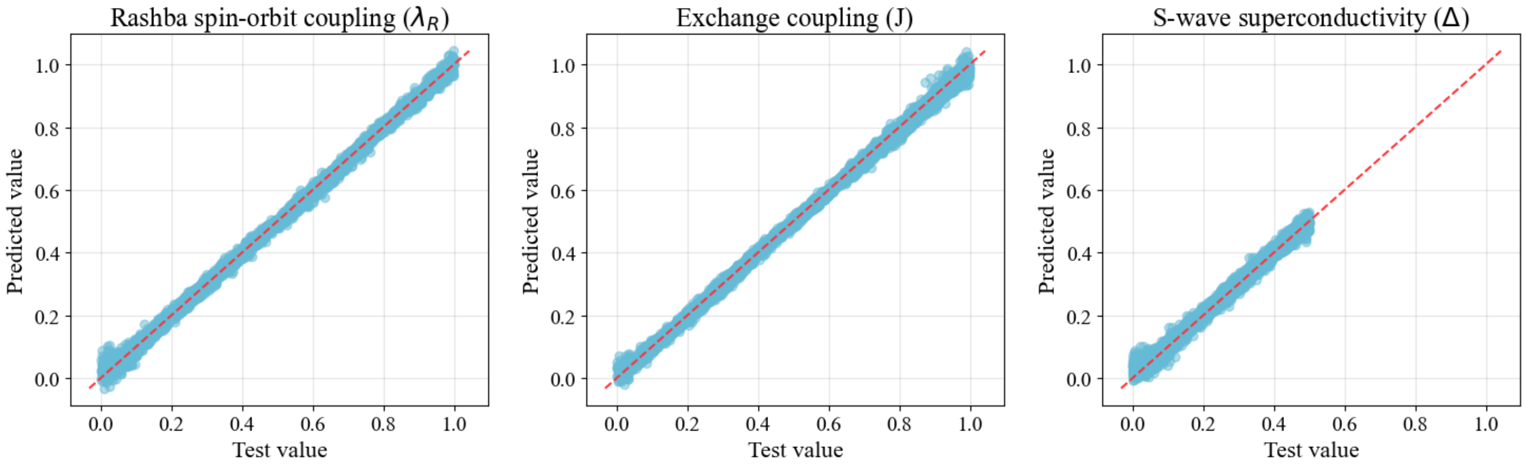
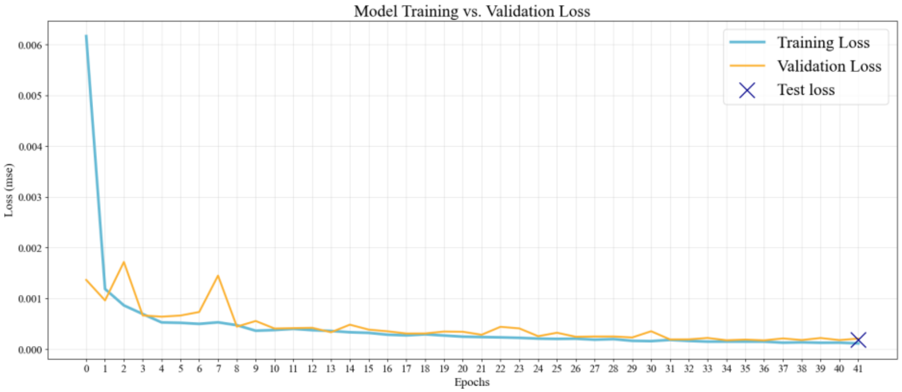
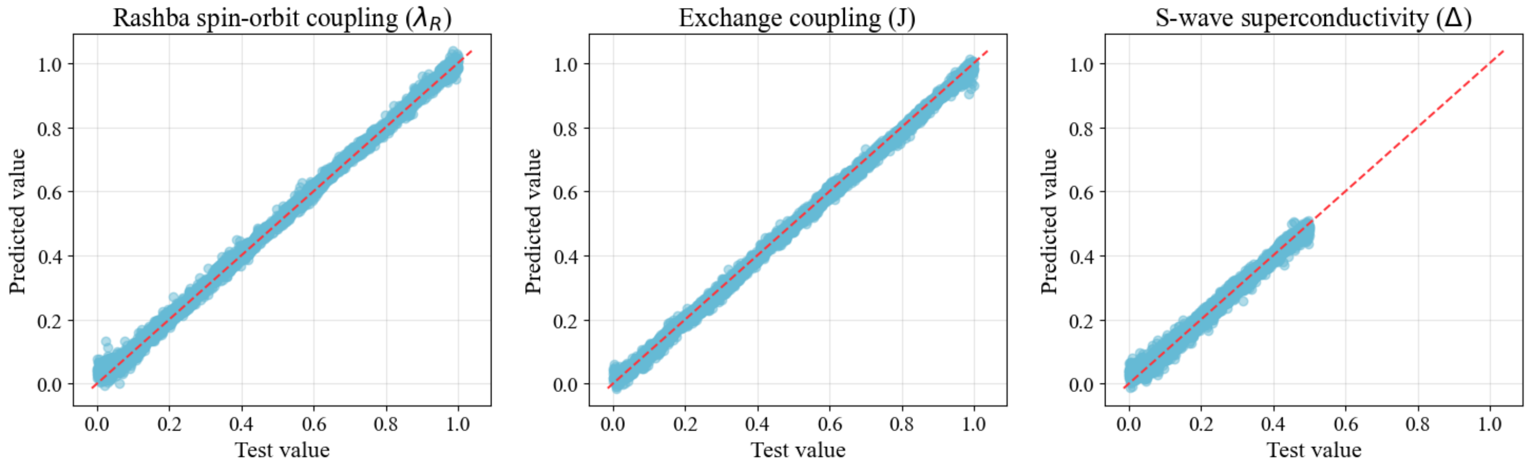
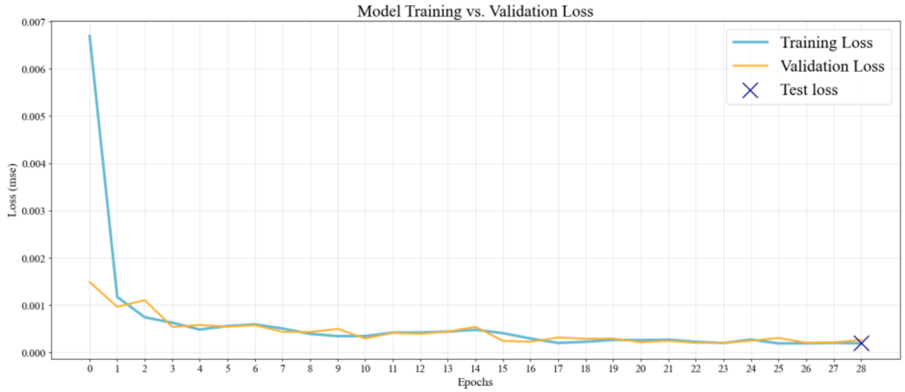




10 site system

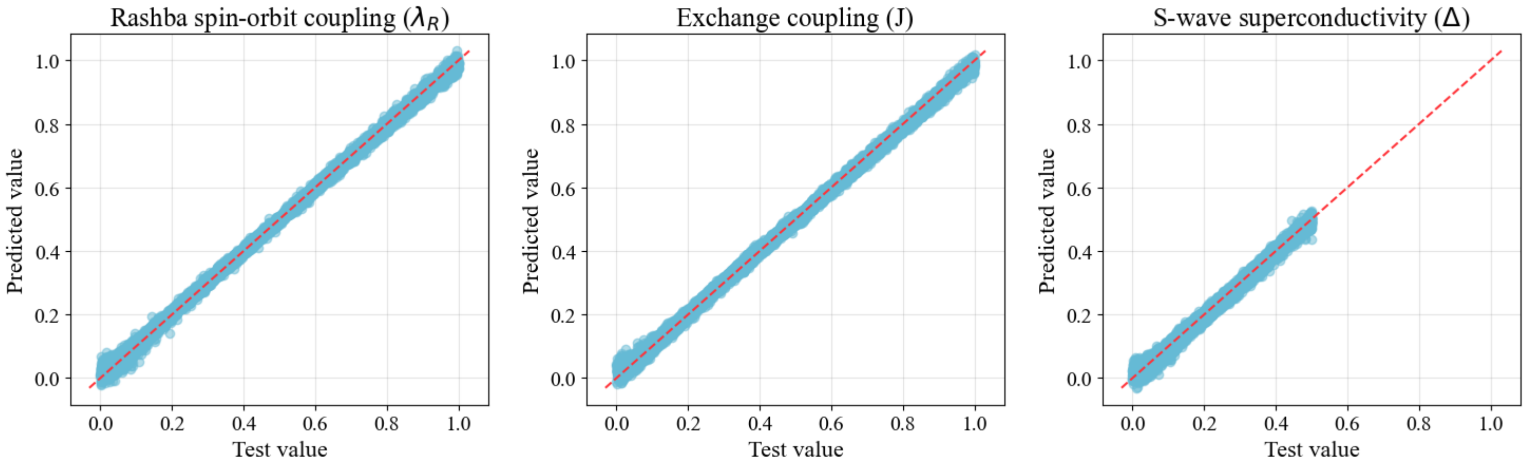
Data compression using PCA: input space reduced to 900,
20 000 Hamiltonians, 20/80 split





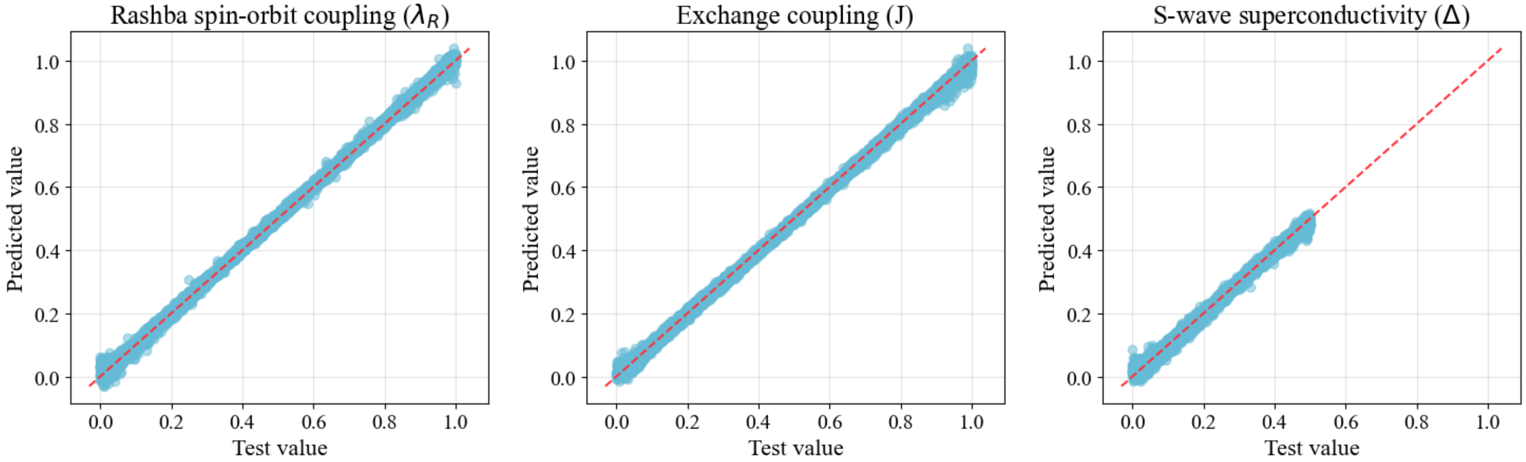
30 site system

No data compression: input space of size 7500,
40 000 Hamiltonians 20/80 split



30 site system

Data compression using PCA: input space reduced to 1500,
40 000 Hamiltonians, 20/80 split



Results

- **It is possible to train a NN model to recognise superconductivity and electron pairing from real-space conductance (DOS) measurements**
- PCA can be used to reduce dimensionality and obtain accurate results faster, but not necessarily to improve results
- A bigger dataset with more training examples could improve the results further, but simulating the data and training the model gets more computationally demanding as the input space grows

References

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